Solid-state Synthesis, Crystal and Band Structures, and Optical Properties of a Novel Ternary Sulfide $Eu_2Ga_2S_5$

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ABSTRACT One new ternary europium gallium sulfide, $Eu_2Ga_2S_5$, has been synthesized by a facile solid-state route with boron as the reducing reagent. It crystallizes in the orthorhombic space group *Pbca*, with a = 11.976(1), b = 11.074 (1), c = 17.446(1) Å, V = 1650.6(3) $Å^3$, and Z = 8. Its 3-*D* structure is built by the connection between EuS_7 monocapped trigonal prisms and GaS_4 tetrahedra, and the latter connect with each other to form layer-like slabs. Its optical energy gap is determined to be 2.17 eV, which is also verified by the electronic band structure calculation.

Keywords: rare-earth sulfide;solid-state reaction;crystal structure, band gap;

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1 INTRODUCTION

Rare-earth chalcogenides have received more attention in recent years in view of their rich crystal structures and diverse physical properties[1, 2]. To date, many rare-earth chalcogenides have been investigated as second-order nonlinear optical[3–5], photocatalytic[6], voltage-dependent[7], and magnetic materials[8, 9]. Encouraged by these applications, exploration on novel rare-earth chalcogenides are still meaningful.

Among rare-earth metals, divalent Eu and Yb ions have similar ionic radii and coordination geometries with alkali-earth metal ions, which make them different from the other trivalent rare-earth metal ions[10]. Recently, many alkali-earth metal chalcogenides have been studied extensively, especially for Ba, Sr-based ones, such as $BaGa_4S_7$[11], $BaGa_2SnSe_6$[12], $Ba_2Ga_8MS_{16}$ (M = Si, Ge)[13], and $BaCdSnS_4$[14]. Most of these compounds are investigated as second-order nonlinear optical materials in the middle and far-infrared region. It should be interesting if Eu^{2+} ions can substitute the II^{2+} (II = Mg, Ca, Sr, Ba) ions in the structures of alkali-earth metal chalcogenides. These Eu-based chalcogenides can be expected to have not only similar physical properties with alkali-earth metal chalcogenides, but also magnetic and photoluminescent properties

because of the existence of *f* electrons. In fact, there are already many such compounds having been reported, such as $EuZrS_3$[15] and $EuGa_2S_4$[16]. When checking the ICSD and Pearson's Handbook, there are a large number of compounds with the formulae $II_2III_2Q_5$ (III = B, Al, Ga, In; Q = S, Se)[17–21] reported. It might be possible to obtain $Eu_2III_2Q_5$ compounds according to the above considerations. On our ongoing exploration on this supposition, one $Eu_2III_2Q_5$ compound, $Eu_2Ga_2S_5$, was obtained. Here, its synthesis, crystal structure, bandstructure, and optical property are presented.

2 EXPERIMENTAL

2. 1 Synthesis and analyses

All starting materials were used as received without further purification. Single crystals of the title compound were obtained by solid-state reaction with KI as flux[22–26]. The starting materials are Eu_2O_3 (99.9%), Ga_2O_3 (99.9%), S (99.999%), and additional boron powder (99%). The sample has a total mass of 500 mg and 400 mg KI (99%) additional, and the molar ratio of Eu:Ga:S:B is 2:2:5:4. The mixture of starting materials was ground into fine powder in an agate mortar and pressed into one pellet, followed by being loaded into one quartz tube. The tube was evacuated to be 1×10^{-4} torr and flame-sealed. The sample was placed into muffle furnace, heated from room temperature to 573 K in 5 h, kept at 573 K for 10 h, then heated to 923 K in 5 h, kept at 923 K for 10 h, then heated to 1223 K in 5 h, kept at 1223 K for 7 days, finally cooled down to 573 K in 5 days, and powered off. The block brown crystals of $Eu_2Ga_2S_5$ stable in air and water were obtained. Semiquantitative microscope elemental analyses on several single crystals were performed on a field-emission scanning electron microscope (FESEM, Hitachi S-4800II) equipped with an energy dispersive X-ray spectroscope (EDS, Bruker, Quantax), which confirmed the presence of Eu, Ga, and S with the approximate molar ratio of 1.95:2.03:5.10 (Fig. 1), and no other elements were detected. The exact composition was established from the X-ray structure determination.

2. 2 Structure determination

The intensity data sets were collected on a Bruker D8 QUEST diffractometer with graphite-monochromated Mo-$K\alpha$ radiation (λ = 0.71073 Å). The structure of $Eu_2Ga_2S_5$ was solved by direct methods and refined by full-matrix least-squares techniques on F^2 with anisotropic thermal parameters for all atoms. All the calculations were performed using Shelxtl-2014[27] through the Olex2[28] interface. The final refinements included anisotropic displacement parameters for all atoms and a secondary extinction correction.

$Eu_2Ga_2S_5$ is crystallized in the orthorhombic space group *Pbca* with Z = 8, a = 11.976(1), b = 11.074 (1), c = 17.446(1) Å, and V = 1650.6(3) Å^3. The final R and wR values for all data are 0.0307 and 0.0425, respectively. The bond lengths are listed in Table 1.

2. 3 Optical properties

The infrared (IR) spectrum was recorded by using a TENSOR27 FT-IR spectrophotometer in the range of 400～4000 cm^{-1}. Powdery sample was pressed into one pellet with KBr. The diffuse reflectance spectrum was recorded at room temperature on a computer-controlled Varian Cary 5000 UV-Vis-NIR spectrometer equipped with an integrating sphere. The measurement wavelength was set in the range of 300～1700 nm. A $BaSO_4$ plate was used as a reference, on which the finely ground powdery sample was coated. The absorption spectrum was calculated from reflection spectrum by the Kubelka-Munk function.

2. 4 Theory calculation

The calculation model was built directly from the single-crystal structure data of $Eu_2Ga_2S_5$. Its electronic band structure based on density functional theory (DFT) was performed using software Material Studio[29]. The generalized gradient approximation (GGA) was chosen as the exchange-correlation functional and a plane wave basis with the projector-augmented wave (PAW) potentials was used. The plane-wave cutoff energy of 480 eV and the threshold of 10^{-5} eV were set for the self-consistent-field convergence of the total electronic energy. The electronic configurations for Eu, Ga and S were 5*d* and 4*f*, 4*s* and 4*p*, and 3*s* and 3*p*, respectively. The numerical integration of the Brillouin zone was performed using 4 × 4 × 4 Monkhorst-Pack *k*-point meshes and the Fermi level (E_f = 0 eV) was selected as the reference.

3 RESULTS AND DISCUSSION

$Eu_2Ga_2S_5$ is crystallized in the orthorhombic space group *Pbca* (No. 61), belonging to the $Mg_2Al_2Se_5$ structure type. There are two Eu (Eu(1) and Eu(2)), two Ga (Ga(1) and Ga(2)), and five S atoms in the crystallographically independent unit. Its structure is composed of two structural units, namely, EuS_7 monocapped trigonal prism (*mtp*) and GaS_4 tetrahedron (Fig. 2), in which all the Eu, Ga and S atoms occupy the 8*c* sites.

The 3-*D* structure of $Eu_2Ga_2S_5$ is constructed by the connection between EuS_7 *mtps* and GaS_4 tetrahedra (Fig. 3). In fact, Ga(1)S_4 and Ga(2)S_4 tetrahedra connect with each other to form layer-like slabs parallel to the *ac* plane (Fig. 4), and Eu(1) and Eu(2) atoms occupy the interlayer monocapped trigonal prismatic cavities.

The 2-*D* slab features a cluster built by four Ga(1)S_4 and four Ga(2)S_4 tetrahedra as the cluster circled in Fig. 4. This polyanionic cluster can be formulated as $[Ga_8S_{20}]^{16-}$ as only one S atom (S(5) for Ga(1)S_4 tetrahedron and S(3) for Ga(2)S_4 tetrahedron) in each GaS_4 tetrahedron has no connection with the other ones, while each of the other three S atoms is shared by two neighboring GaS_4 tetrahedra. It can be observed that Ga(1)S_4 and Ga(2)S_4 tetrahedra are connected alternatingly via sharing S corners. Each such cluster has four neighboring $[Ga_8S_{20}]^{16-}$ clusters.

The Eu–S bond distances in $Eu_2Ga_2S_5$ are in the range of 2.927(2)～3.227(2) Å, which are in good agreement with those of the corresponding compounds in literatures[15, 16]. The Ga–S bond lengths in the range of 2.221(2)～2.334(2) Å are consistent with those found in $(K_3I)[SmB_{12}(GaS_4)_3]$[5], $EuGa_2S_4$[16], and $BaGa_2S_5$[18].

The $II_2III_2Q_5$ (II = Mg, Ca, Sr, Ba; III = B, Al, Ga, In; Q = S, Se) family compounds have been extensively investigated for a long time[17–21]. The known members include $Mg_2Al_2Se_5$, $Sr_2Ga_2S_5$, $Ba_2Ga_2S_5$, and $Ba_2In_2Q_5$ (Q = S, Se). Most of the previous reports only studied their crystal structures, and only S. L. Pan recently has reported the electronic structures and optical properties of $Ba_2In_2Q_5$[21]. It is surprising that there is no investigation on $Eu_2III_2Q_5$ compounds until now. Since one Eu^{2+} ion contains seven *f* electrons, largely different from the II^{2+} ions, it is more attractive to investigate the versatile physical properties of Eu-based chalcogenides.

Except for $II_2III_2Q_5$ compounds, some oxide variants of them have also been reported. Lots of $II_2III_2O_5$, including $Mg_2B_2O_5$, $Ca_2B_2O_5$, $Mg_2Al_2O_5$, $Ca_2Al_2O_5$, $Ba_2In_2O_5$, and $Sr_2Ga_2O_5$[30–33], have been studied.

Moreover, two III atoms in $II_2III_2Q_5$ can be substituted by one divalent and one tetravalent atoms, respectively, such as Ba_3GeS_5. If introducing transition metal atom to replace one of the two II atoms in $II_2III_2Q_5$, several quaternary variants can be obtained, and the known examples include $BaLn_2MS_5$ (Ln = rare-earth metal; M = Mn, Fe, Co, Zn) and $BaLa_2Co(S_{1-x}Se_x)_5$[34–37].

The IR and diffuse reflection spectra of $Eu_2Ga_2S_5$ are shown in Figs. 5 and 6. Indeed, the measurement results show that $Eu_2Ga_2S_5$ is transparent in the IR range of 400～4000 cm^{-1} (2.5～25 μm), and an optical band gap of 2.17 eV, which is consistent with its brown color.

To investigate the electronic structures of $Eu_2Ga_2S_5$, its bandstructure computation based on the DFT theory was performed using CASTEP mode in Material Studio software[29]. The calculated band structure along high symmetry points of the first Brillouin zone is shown in Fig. 7, from which it can be seen that the band gap of $Eu_2Ga_2S_5$ is calculated to be 2.21 eV, which is reasonable in view of the calculation precision.

Both the lowest conduction band (CB) and the highest valence band (VB) of $Eu_2Ga_2S_5$ are located at G point, indicating that it has a direct band gap.

In conclusion, a new ternary Eu-based sulfide $Eu_2Ga_2S_5$ was obtained using high-temperature solid-state reaction. Its optical properties indicate that it may be used as IR window materials, and also have some potential applications in the fields of photoelectric materials in view of its direct band gap. It is supposed that more Eu^{2+} ion substituted $II_2III_2Q_5$ (II = Mg, Ca, Sr, Ba; III = B, Al, Ga, In; Q = S, Se) compounds can be discovered.

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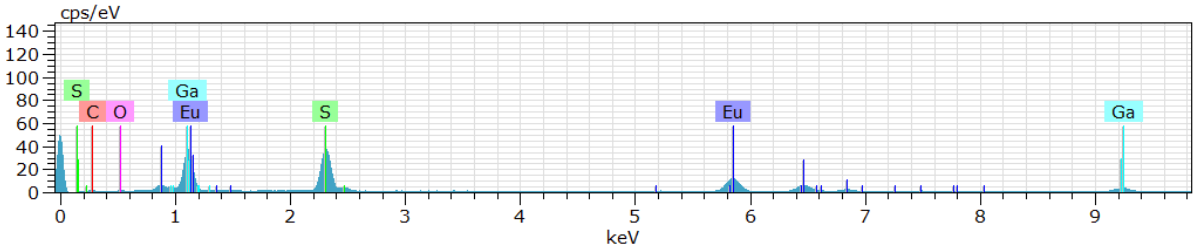
Table 1. Bond Lengths for $Eu_2Ga_2S_5$

Bond	Dist.	Bond	Dist.
Eu(1)–S(1)#7	2.945(2)	Eu(2)–S(4)#5	3.162(2)
Eu(1)–S(1)#6	3.178(2)	Eu(2)–S(5)#5	3.113(2)
Eu(1)–S(2)#4	3.227(2)	Eu(2)–S(5)#9	3.157(2)
Eu(1)–S(3)	3.146(2)	Ga(1)–S(1)#2	2.334(2)
Eu(1)–S(3)#6	3.039(2)	Ga(1)–S(2)	2.277(2)
Eu(1)–S(5)	2.927(2)	Ga(1)–S(4)	2.290(2)
Eu(1)–S(5)#5	2.930(2)	Ga(1)–S(5)	2.245(2)
Eu(2)–S(1)#8	3.132(2)	Ga(2)–S(1)	2.330(2)
Eu(2)–S(2)#7	3.054(2)	Ga(2)–S(2)	2.290(2)
Eu(2)–S(3)	2.954(2)	Ga(2)–S(3)	2.221(2)
Eu(2)–S(3)#9	3.052(2)	Ga(2)–S(4)#4	2.296(2)

Symmetry transformations used to generate the equivalent atoms: #1 1–*x*, –1/2+*y*, 1/2–*z*; #2 3/2–*x*, –1/2+*y*, *z*; #3 *x*, 3/2–*y*, 1/2+*z*; #4 1–*x*, 1–*y*, 1–*z*; #5 1–*x*, 1/2+*y*, 1/2–*z*; #6 –1/2+*x*, y, 1/2–*z*; #7 3/2–*x*, 1–*y*, –1/2+*z*; #8 *x*, 3/2–*y*, –1/2+*z*; #9 3/2–*x*, 1/2+*y*, *z*; #10 1/2+*x*, *y*, 1/2–*z*; #11 3/2–*x*, 1–*y*, 1/2+*z*

Fig. 1. EDS analysis of $Eu_2Ga_2S_5$



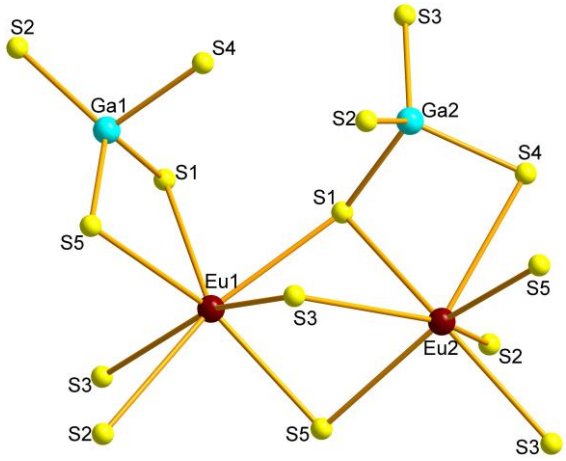


Fig. 2. Coordination geometry of $Eu_2Ga_2S_5$

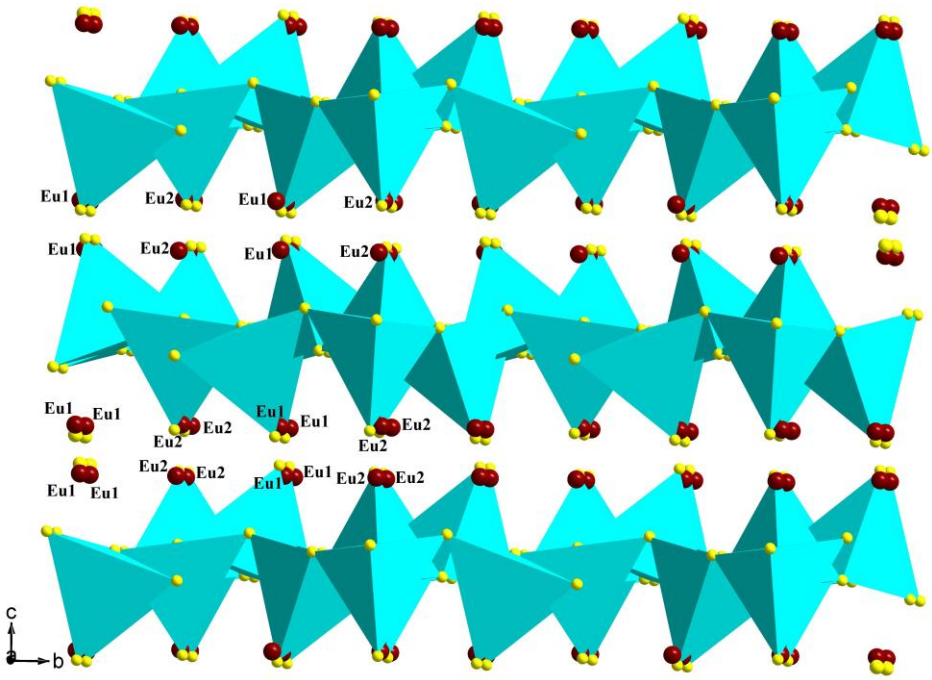


Fig. 3. 3-*D* crystal structure of $Eu_2Ga_2S_5$ constructed by the connection between GaS_4 tetrahedra (blue) viewed along the *a* direction, where the Eu–S bonds are omitted for clarity

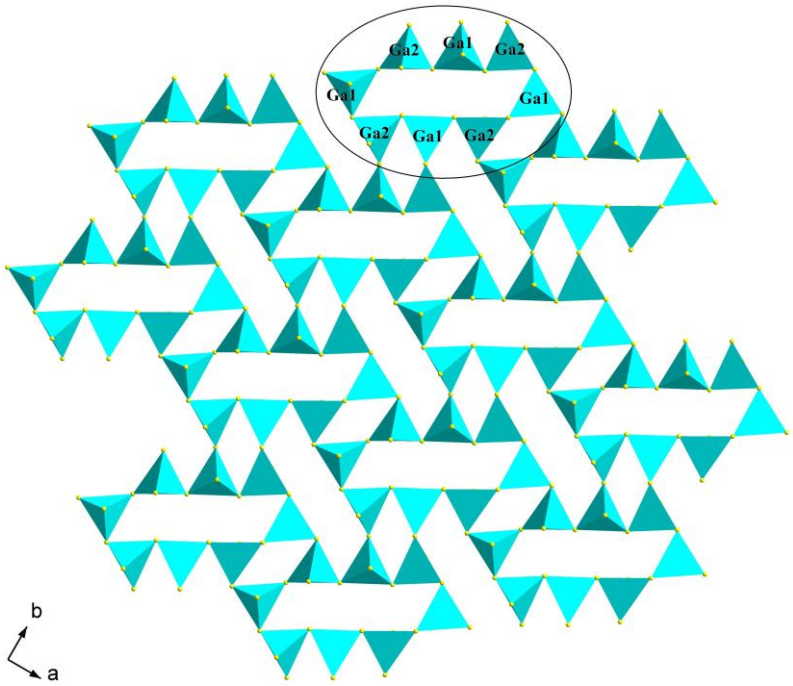


Fig. 4. Connection between GaS_4 tetrahedra in the crystal structure of $Eu_2Ga_2S_5$ viewed parallelly to the *ab* plane

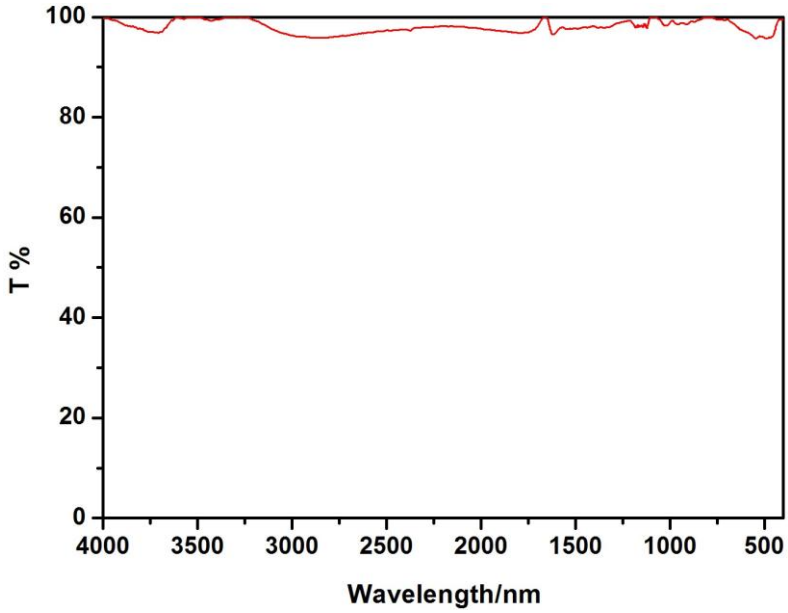


Fig. 5. IR spectrum of $Eu_2Ga_2S_5$

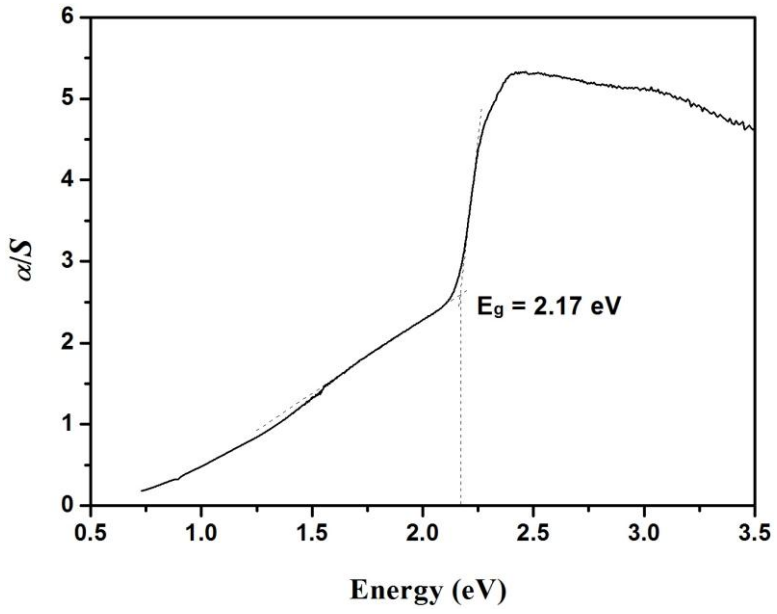


Fig. 6. Diffuse reflection spectrum of $Eu_2Ga_2S_5$

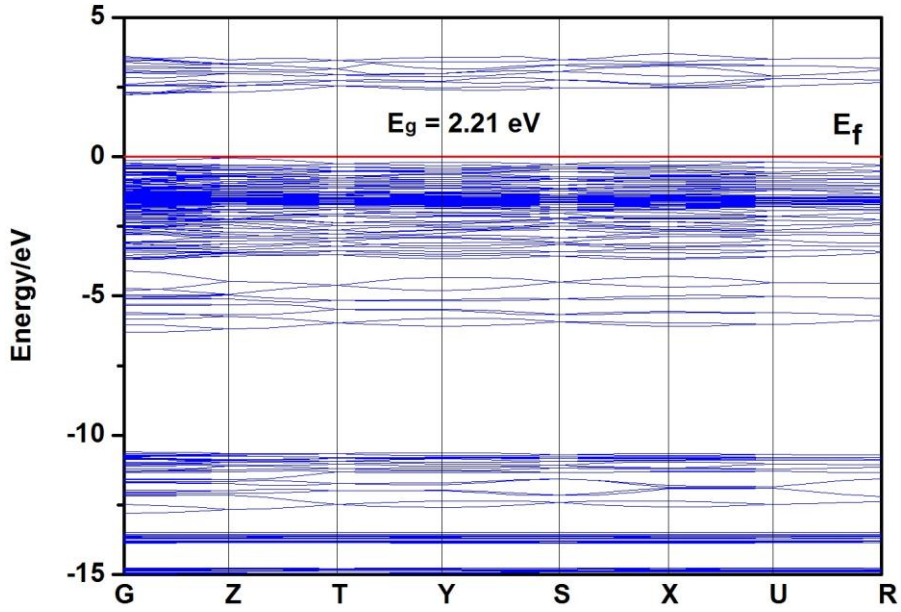


Fig. 7. Calculated band structure of $Eu_2Ga_2S_5$.

The Fermi level is chosen as the energy reference at 0 eV and the band gap is calculated to be 2.21 eV

Solid-state Synthesis, Crystal and Band Structures, and Optical Properties of a Novel Ternary Sulfide $Eu_2Ga_2S_5$

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One new ternary europium gallium sulfide, $Eu_2Ga_2S_5$, has been synthesized by a facile solid-state route. It crystallizes in the orthorhombic space group *Pbca*, and its 3-*D* structure is built by the connection between EuS_7 monocapped trigonal prisms and GaS_4 tetrahedra, and the latter connect with each other to form layer-like slabs. Its optical energy gap is determined to be 2.17 eV, which is also verified by the electronic band structure calculation.